Post-Gaussian variational method for quantum anharmonic oscillator

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Abstract

Using the post-Gaussian trial functions, we calculate the variational solutions to the quantum-mechanical anharmonic oscillator. We evaluate not only the ground state but also some excited energies, and compare them with numerical results.

1. INTRODUCTION

The post-Gaussian trial function provides a robust instrument for obtaining the variational solutions[1,2] . By using the post-Gaussian trial function, one gets an excellent estimate for the ground-state of the system. These results indicate the possibility for obtaining better solutions for the potential problems, not only the ground state but also the excited states.

In this article, we examine the utility of the post-Gaussian trial wave functions. For this purpose, we employ the anharmonic oscillator as an example. The anharmonic oscillator has been given the useful laboratory to test a nonperturbative approximation. We also show explicitly that the post-Gaussian variational method gives better solutions to the anharmonic oscillator than the ordinary Gaussian one. This may give insight into a quantum-field-theoretical problem in the standard Gaussian variational approach to spontaneous symmetry breakings.

In the following section, we solve the ground-state energy of the anharmonic oscillator

using the variational method with post-Gaussian trial wave function. In section 3, we calculate some excited-state energy levels and compare the results with numerical calculations. Section 4 is devoted to discussions. Throughout this paper all quantities and variables are assumed to be made dimensionless for simplicity.

2. POST-GAUSSIAN VARIATIONAL METHOD AND THE GROUND STATE

The system we consider is the anharmonic oscillator. The Hamiltonian is written as follows:

$$H = \frac{p^2}{2} + \frac{x^2}{2} + gx^4, \tag{1}$$

where g is a positive constant.

To obtain the ground-state energy of H using the variational method, we employ a post-Gaussian trial function [1,2] :

$$\psi^{(0)} = \mathcal{N}^{(0)} \exp\left[-\frac{\alpha}{2}|x|^{2n}\right], \tag{2}$$

where the normalization constant $\mathcal{N}^{(0)}$ is given by

$$\mathcal{N}^{(0)} = \sqrt{\frac{n\alpha^{\frac{1}{2n}}}{\Gamma(\frac{1}{2n})}}. \tag{3}$$

$\Gamma(z)$ is Euler's gamma function of argument z. We notice that this trial function in Eq.(2) has two variational parameters; i.e. α and n. In the case of $n = 1$, this trial function reduces to the familiar Gaussian trial function which is often taught in an elementary course of quantum mechanics.

Using Eq.(2), we calculate the expectation value of the Hamiltonain as follows:

$$I^{(0)}(\alpha, n) \equiv \langle\psi^{(0)}(n,\alpha)|H|\psi^{(0)}(n,\alpha)\rangle \tag{4}$$

$$= \frac{n^2}{2}\frac{\Gamma(2-\frac{1}{2n})}{\Gamma(\frac{1}{2n})}\alpha^{1/n} + \frac{1}{2}\frac{\Gamma(\frac{3}{2n})}{\Gamma(\frac{1}{2n})}\alpha^{-1/n} + g\frac{\Gamma(\frac{5}{2n})}{\Gamma(\frac{1}{2n})}\alpha^{-2/n}. \tag{5}$$

The optimization of Eq.(5) with respect to the two parameters α and n

$$\left.\frac{\partial I^{(0)}}{\partial\alpha}\right|_{\alpha_0} = 0, \tag{6}$$

$$\left.\frac{\partial I^{(0)}}{\partial n}\right|_{n_0} = 0, \tag{7}$$

can easily accomplished numerically.

In Table 1., we show the numerical result for the ground state. The optimal value is found to be at $n = n_0 = 1.13493$ that indicates the wave function deviates from the Gaussian one.

3. THE EXCITED STATES AND THE NUMERICAL RESULTS

The first excited state $\psi^{(1)}$ can be determind in such a way that the following orthogonality condition is satisfied:

$$< \psi^{(0)}(n_0, \alpha_0)|\psi^{(1)}(n_0, \beta) >= 0, \tag{8}$$

where n_0 and α_0 are fixed values of the variational parameters obtained in the previous section and β is a new variational parameter. Then, using this trial function, we optimize the expectation value of the Hamiltonian:

$$I^{(1)}(\beta, n_0) =< \psi^{(1)}(n_0, \beta)|H|\psi^{(1)}(n_0, \beta) > . \tag{9}$$

To find the second excited state, we again optimize the expectation value of the Hamiltonian using another trial function $\psi^{(2)}$ which is orthogonal to both $\psi^{(0)}$ and $\psi^{(1)}$:

$$< \psi^{(0)}(n_0, \alpha_0)|\psi^{(2)}(n_0, \gamma) >= 0, \quad < \psi^{(1)}(n_0, \beta_0)|\psi^{(2)}(n_0, \gamma) >= 0, \tag{10}$$

where β_0 is the fixed value which make Eq.(9) optimal and γ is again a new variational parameter. The same procedure stated above can repeatedly be applied to find the higher excited states.

Now, inspired by the harmonic-oscillator wave functions, we propose to take the following trial functions for the excited states:

$$\psi^{(1)} = \mathcal{N}^{(1)} x \exp\left[-\frac{\beta}{2}|x|^{2n_0}\right], \quad \mathcal{N}^{(1)} = \sqrt{\frac{n_0 \beta^{\frac{3}{2n_0}}}{\Gamma(\frac{3}{2n_0})}}, \tag{11}$$

$$\psi^{(2)} = \mathcal{N}^{(2)} \left\{n_0(\alpha_0 + \gamma)|x|^{2n_0} - 1\right\} \exp\left[-\frac{\gamma}{2}|x|^{2n_0}\right],$$

$$\mathcal{N}^{(2)} = \sqrt{\frac{4n_0}{\Gamma(\frac{1}{2n_0})} \frac{\gamma^{2+\frac{1}{2n_0}}}{(2n_0+1)\gamma^2 + 2(2n_0-1)\alpha_0\gamma + (2n_0+1)\alpha_0^2}} \tag{12}$$

In Table 1., we compare the results of the post-Gaussian trial functions with the Gaussian and numerical results[3]. As can explicitly be seen, the post-Gaussian trial functions always give better results than those with the Gaussian trial functions.

4. CONCLUSIONS

We have applied the post-Gaussian trial functions to the anharmonic oscillators. We have explicitly calculated up to the second excited state and compared the results with numerical calculations. We have seen how the post-Gaussian trial functions give the better results than the Gaussian wavefunctions.

Finally, we note that Cooper et al.[4,5] have also discussed the variational energy eigenvalues for the anharmonic oscillator using the post-Gaussian trial functions. Their algorithm to obtain the excited states is based on the idea of SUSY quantum mechanics[6], whereas the method we discussed here is the standard one known in elementary quantum mechanics.

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REFERENCES

1. F. Cooper, H. Shepard, C. Lucheroni and P. Sodano Physica D **68**, 344(1993)

2. F. Cooper, C. Lucheroni, H. Shepard and P. Sodano Phys.Lett. A **173**, 33(1993)

3. F. T. Hioe and E. W. Montroll J.Math.Phys. **16**, 1945(1975)

4. F. Cooper, J. Dawson and H. Shepard Phys.Lett. A **187**, 140(1994)

5. F. Cooper, A. Khare and U. Sukhatme Phys.Rep. **251**, 267(1995)

6. E. Gozzi, M. Reuter and W. D. Thacker Phys.Lett. A **183**, 29(1993)

TABLES

Table 1. Energy eigenvalues of the anharmonic oscillator with $g = 1$ in the Gaussian and post-Gaussian variational methods in comparison with the numerical results. All quantities are dimensionless.

	Gaussian(n=1)	post-Gaussian	numerical
ground	0.81250 (α_0=2.00000)	0.80490 $\begin{pmatrix} \alpha_0 = 1.86647 \\ n_0 = 1.13493 \end{pmatrix}$	0.80377
1st excited	2.75994 (β_0=2.30891)	2.73992 (β_0 = 2.03260)	2.73789
2nd excited	5.21980 (γ_0=2.54205)	5.20002 (γ_0= 2.34411)	5.17929